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Visualization of Polymer Processing at the Continuum Level

Jeremy Hicks
Clemson University, jlhicks@clemson.edu

VISUALIZATION OF POLYMER PROCESSING AT THE CONTINUUM LEVEL

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Jeremy L. Hicks
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Accepted by:
Dr. Timothy Davis, Committee Chair
Dr. John Kundert-Gibbs
Dr. Christopher Cox

ABSTRACT

Computer animation, coupled with scientific experimentation and modeling, allows scientists to produce detailed visualizations that potentially enable more comprehensive perception of physical phenomena and ultimately, new discoveries. With the use of Maya, an animation and modeling program that incorporates the natural laws of physics to control the behavior of virtual objects in computer animation, data from the modeling of physical processes such as polymer fibers and films can be explored in the visual realm. Currently, few attempts have been made at the continuum level to represent polymer properties via computer animation using advanced graphics. As a result, scientists may be unable to recognize patterns and trends in a specific polymer quickly and efficiently, and thus, lose time and money commonly required for further experiments. In this paper, the relationship of dynamic quantities, such as velocity, temperature, crystallinity, and tensile stress of polymers, are visualized through speed, color, surface texture, and shape, respectively, with the use of animated glyphs created in Maya. This method ultimately allows users to better understand the properties of complex fluids, such as polymers, exhibited at multiple scale levels in a more aesthetically pleasing and intuitive fashion. Although we represent scientific data, a secondary objective is to present the information from a more artistic approach, as we introduce the continuum level process from an abstract perspective.

DEDICATION

This work is dedicated to Willie and Ammie Hicks, my beloved parents. You have always supported me in my education, and I am grateful to call you dad and mom. To Shineka Morris, I am truly blessed to have you as my sister. I also dedicate this work to the younger generation. Keep the faith!

ACKNOWLEDGMENTS

I would like to thank my advisor, Dr. Timothy Davis, for his encouragement, support, and guidance during the completion of this degree.

Dr. Kundert-Gibbs introduced me to the exciting and intriguing world of computer animation. I am grateful for his instruction and expertise.

I would like to thank Dr. Chris Cox for giving me the opportunity to work for the Center For Advanced Engineering Fibers and Film. Through your leadership and direction, I have been able to contribute to the ongoing research of polymer science.

Stanley Sims, Chris Doeling, Serenthia Ross, and Professor Tony Penna were very helpful throughout my graduate career.

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CHAPTER 1

INTRODUCTION

For quite some time, computer animation has been evolving beyond the film industry to the advertisement, gaming, and television arenas, where it serves as a communication enhancement. Another area where this form of art presents exciting possibilities is in science and technology. With new discoveries achieved daily in these fields, researchers are able to make more accurate predictions concerning physical phenomena through the use of high-end graphics. Scientific principles that are not fully understood, such as those exhibited in polymer processing, can also be explored using computer animation.

For many decades, intense research has been devoted to the advancement of polymer science. Scientists seek to impose a desired shape and final properties on a particular polymer, thereby increasing the value of the product. For example, the body and wings of the F-117A stealth fighter/bomber are created using an epoxy/carbon fiber composite which is produced using a process called hand lay-up [POLY06]. This method allows for detailed control of fiber orientation at different locations on the part. The materials used in this process are preprocessed in the shape of flat sheets that consist of a uniaxial carbon fiber. These sheets, which have a low or medium molecular weight epoxy, are then molded into the desired shape of the wings. As a result of its high strength to weight ratio, the wing is able to support the loads that are expected to be generated during flight. Also, since the materials have low reflection compared to metals,

the aircraft exhibits higher stealth characteristics in battle. Thus, the choice of materials and the process to create this polymer product are critical for achievement of the desired performance. However, producing this highly sophisticated stealth aircraft costs money and time. High performance epoxy/carbon composites are very costly, and it is imperative to have a large amount of highly trained labor in the hand lay-up process; thus, improving upon certain methods of polymer production to promote economic savings is essential. For this reason, computer animation coupled with modeling can serve as an enhancement, as it allows researchers to better understand the structure and properties of polymers such as those found in the F-117A stealth fighter/bomber. Ultimately, this knowledge may result in new discoveries and advances in the polymer industry with significantly reduced cost of experimentation.

In this paper, we will describe an animation in Maya illuminating the relationship of dynamic quantities of polymers at the continuum level. Some of the properties that will be explored are velocity, temperature, crystallinity, and tensile stress. To represent these elements, we will create animated glyphs in the shape of spheres. These primitives will change over time with respect to speed, color, texture, and shape to illustrate velocity, temperature, crystallinity, and tensile stress, respectively. Our goal will be to create this visualization as accurately as possible. To accomplish this task, we will use real 2D data images from a particular polymer as references. This visualization will hopefully contribute to the ultimate goal of allowing users to better understand the properties of complex fluids at multiple scale levels in a more aesthetically pleasing and intuitive fashion.

In Chapter 2, we give a more in-depth analysis of polymers and their importance

in everyday life. In Chapter 3, we describe related work in polymer visualization lacking high-end graphics and how developing a more realistic computer animation enhances the way students, researchers, and industrial workers learn about polymers. We also discuss other abstract animations used to emphasize the aesthetic nature of polymers. In Chapter 4, we present our solution step by step and describe the obstacles encountered in the implementation phase. In addition, we analyze our method and how it contributes to our goal of creating an abstract animation. Images of the final animation are shown in Chapter 5. In Chapter 6, we conclude by discussing contributions of this work and possible future enhancements.

CHAPTER 2

BACKGROUND

Polymers, which are derived form the Greek word *poly* meaning 'many' and *meros* meaning 'parts', can be defined as large molecules consisting of repetitive units connected by covalent chemical bonds [MARK06]. They are fundamental to life, as all living organisms can be identified by their DNA or Deoxyribonucleic acid, which is itself a polymer [DAVI06]. These large repeated chains have a vast range of applications, from the food and drink packages we consume daily to the clothing fabrics we wear.

Today, the polymer industry has outgrown the steel and aluminum businesses combined, and it has made tremendous contributions to the various facets of life. For example, polymeric materials have been involved in agriculture science to improve aeration and promote plant growth. Water crystals, which are polyacrylamide polymers, have been used to absorb water for plants. As these gello-ice cubes submerge in water, the cubes grow to the size of an acorn and hold excess moisture after being placed in soil. The crystals will retain the water for extended periods of time depending on air temperature and the thirst of the plants. Subsequently, the feeder roots of plants drain the sustaining water from the crystal by penetrating the cube's membrane. While being consumed by the roots, the hydrated crystal absorbs neighboring moisture and nutrients from the soil. When the soil is irrigated or drenched by rain, the water crystals fill up with water and thus continue to preserve the plant. These odorless cubes are also less susceptible to mold, bacterial growth, and fungi, which are harmful to plants [WC06].

Overall, these polymers have proven to be one of many successful methods used in protecting plants from both drought and excessive moisture. Figure 2.1 shows a picture of water crystals.

Figure 2.1 Water Crystals used to absorb water for plants [WC06]

Polymer research has contributed to the automotive industry as well. The polymer Polyisobutylene, which is a gasoline additive, has been proven to increase horsepower and mileage in cars. Scientists discovered that smaller hydrocarbons in gas separate from larger ones when placed in the engine's combustion chamber. However, by adding a small percent of polyisobutylene to a tank of gas, gasoline is able to burn more evenly and at a lower temperature, and thus keeps the hydrocarbons together. As a result, fewer hydrocarbons are left unburned and more energy is harvested [HSW06]. In addition, polyisobutylene decreases 70 percent of the emissions in certain environmental pollutants such as carbon monoxide and nitrogen oxides. Another product made of polymers, plastic, has been used in the automotive business to reduce weight in cars. Due to the rise in fuel costs, automotive companies are beginning to look for lightweight technologies. Plastic material can achieve this improvement as it yields an increase in

fuel economy. In contrast to stamping steel, plastic can also be shaped into far more complex shapes. Thus, a single- injected molded plastic part can accomplish just as much as many metal pieces joined together [ALEX06]. As Figure 2.2 illustrates, polymers are found in other auto parts.

Figure 2.2 Seats in automobiles made of plastic [ALEX06]

Molecular shape and the way molecules are assembled are essential factors in determining the properties of a polymer. For example, the way spaghetti noodles lay on a plate can be compared to how a polymer appears in an amorphous state, in which the arrangement of molecules has no definite form. As a result, polymer chains have no order to arrange themselves, and thus become tangled. An amorphous polymer, which is generally transparent, is an important state for applications such as food wrap, plastic windows, and contact lenses. Polymer chains in opaque objects are in a crystalline state, in which the arrangement of atoms, ions, and molecules have a distinct pattern. Figure 2.3 shows this comparison between an amorphous and a crystalline state. The degree of crystallinity desired determines the way polymers are produced. The higher the degree of crystallinity, the less light can pass through the material [PLCY06]. This is apparent in

the comparison of ice and glass when viewed between crossed polarizers. Glass, which is an amorphous material, changes the apparent properties of the polarized light. Consequently, glass appears dark because of its unorganized structure, which is in contrast to the highly ordered crystalline structure of ice which appears bright. Crystalline solids also show a definite melting point, unlike amorphous material, and so transition rather sharply from solid to liquid state. In the heating process of amorphous materials, the polymer changes from solid to a viscous or thick liquid. However, the morphology of most polymers is semi-crystalline [PLCY06]. These polymers form mixtures of small crystals and amorphous material and liquefy over a range of temperatures instead of a single melting polymer. The combination of crystalline and amorphous structures allows a polymer to have advantageous properties of strength and stiffness.

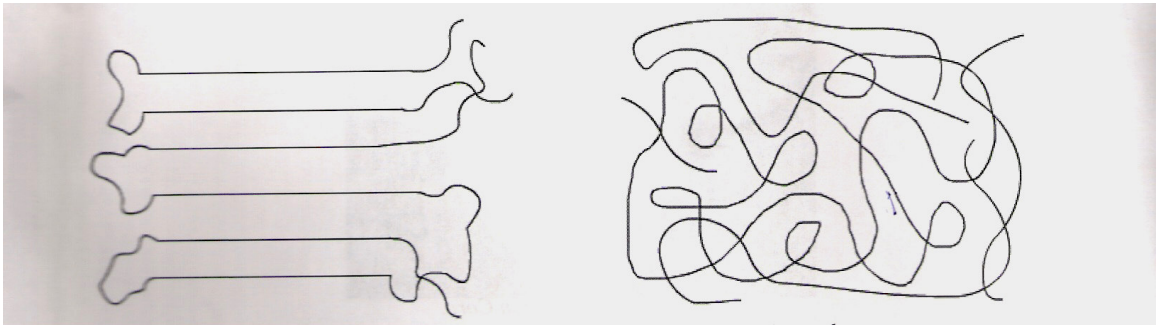


Figure 2.3 A crystalline state is shown to the left of the picture, while an amorphous state is shown to the right [PLCY06]

Viscoelasticity is another facet of the behavior of polymers. To understand this feature, one must be knowledgeable of elasticity, the ability of an object to deform under stress but return to its original shape when the stress is removed [POLI06]. A spring, which can be stretched to a new length but recoils when the stress is removed, is an example of an object exhibiting an elastic behavior. Deformation occurs when stress is applied, and it is totally recovered upon release of the external stress. Polymers, however,

exhibit a viscous effect, which causes the deformations in a material from stress to be time-dependent. The reason for this dependency is the amount of time it takes for applied forces causing bonds in polymer chains to rotate about an axis [POLI06]. If a stress is applied slowly to a polymeric body, the polymer chains have time to stretch and unfold. In this condition, polymers undergo large deformations with little elastic behavior. In contrast, if the stress is applied rapidly, the chains do not have enough time to react, and thus appear more elastic and much less flexible. One example of this phenomenon is a silicone polymer, shown in Figure 2.4. When rolled into a ball and dropped onto a horizontal surface, the material bounces elastically. However, with a gradually increased applied stress, the polymer flows like a highly viscous liquid flow. It should be noted that deformation is not instantaneous for totally viscous behavior and is not reversible or completely recovered after the stress is released for elastic behavior.

Figure 2.4 Silicone Polymer, also known as silly putty, shows viscoelastic behavior as it drips through a hole [WIKI06]

Another interesting, yet complicated, phenomenon occurs in polymers after exiting the die of an extruder model. This experience known as die swell, can be defined

as the enlargement of an extrudate over the dimensions of the die capillary from which it is extruded [KROS87]. As shown in Figure 2.5, a polymeric fluid expands in a radial direction once it is outside the capillary of the die. The swell, also known as extrudate swell, is an indication of the elasticity of a polymer. The more elasticity a polymer possesses, the larger the swell. By pulling the extrudate, the swell is reduced and can be drawn down to diameters much smaller than the diameter of the die capillary.

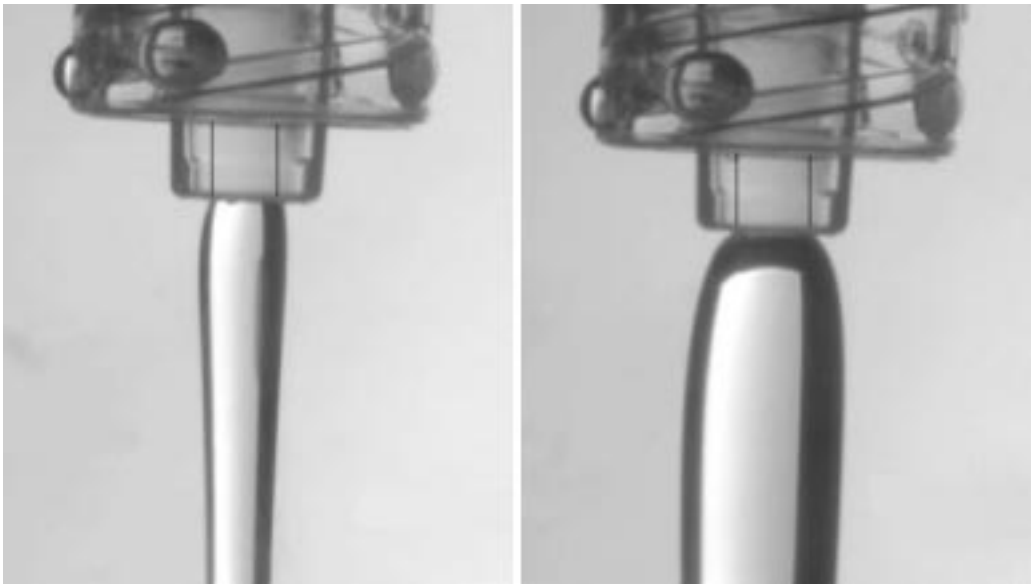


Figure 2.5 Polymeric fluid exhibits a die swell shape as it exits the capillary of the die [MIT06]

Tensile strength is a key element scientists use to determine the robustness of a polymer. Tensile strength is the maximum amount of longitudinal stress, or tensile stress, a substance can bear without breaking apart [MW06]. A polymer's tensile strength depends on the molecular structure of the polymer as well as the orientation of the material. When pulled lengthwise, these molecular chains can elongate a great distance before tearing. However, when pulled widthwise, only the entanglements hold the polymer together. Thus, the polymer is more likely to break in this direction. There are

three typical definitions of tensile strength – yield, ultimate, and break [WIKI06]. Yield strength is the stress a material can endure without permanent deformation; ultimate strength is the maximum stress a material can undergo; and break strength is the stress coordinates on the stress-strain curve at the point of rupture.

In the next chapter, we discuss related work in polymer visualization and compare our animation to these modules. Also, we present other abstract work used to emphasize molecular beauty and make assessments of the aesthetic nature of these animations and the one we are implementing.

CHAPTER 3

RELATED WORK

Scientific visualization has proven to be a powerful tool in computational science. Section 3.1 discusses such software packages and their contributions to advances in polymer research. We outline some of the advantages and disadvantages of these software tools in Section 3.2. In Section 3.3, we focus our attention on abstract visual animation and how it has been used to capture the beauty inherent in polymer science. We conclude in Section 3.4 by discussing these abstract animations from an artistic perspective and compare the visuals to our work.

3.1 Software Packages

Several packages have allowed users to better understand the results of their experiments.

3.1.1 Maya

Maya, a high-end 3D computer graphics and 3D modeling program, is able to create extraordinary, visual effects and animations [WIKI06]. As shown in Figure 3.1, this software can display geometry as NURBS (Non-Uniform Rational B-Spline), Polygons, or Subdivision Surfaces. Maya, which has amazing rendering and texturing capabilities, also features a powerful, interpreted, cross-platform scripting called Mel Scripting Language.

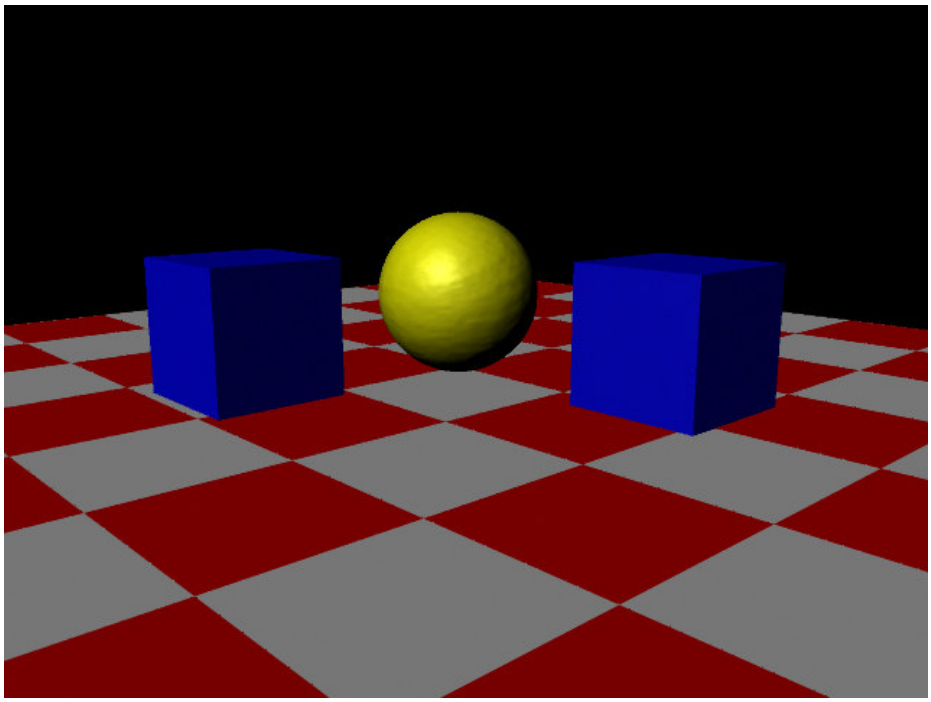


Figure 3.1 Geometry displayed in Maya [WIKI06]

3.1.2 VTK

VTK, also known as the Visualization Toolkit, is a scientific, open-source software application for 3D computer graphics, visualization, and image processing [VT06]. This freely available system, which is used by researchers and engineers around the world, supports a vast majority of visualization algorithms including scalar, vector, and texture methods, as well as modeling techniques such as polygon reduction, mesh smoothing, and contouring. VTK applications can be written in programming languages such as Java, C++, Tcl, and Python, and dozens of imaging algorithms have been directly integrated to allow the user to combine 2D imaging and 3D graphics algorithms and data. By using the interpreted languages such as Tcl and Python, it is even possible to build useful interfaces quickly.

The Center For Advanced Engineering Fibers and Film (CAEFF), a multi-institutional NSF Research Center located on the campus of Clemson University, uses the advanced capabilities of VTK to convert experimental and modeling data into 2D data plots, as shown in Figure 3.2 [CAEF06]. These images have given researchers a better understanding about the different properties of polymers used to make fibers and film.

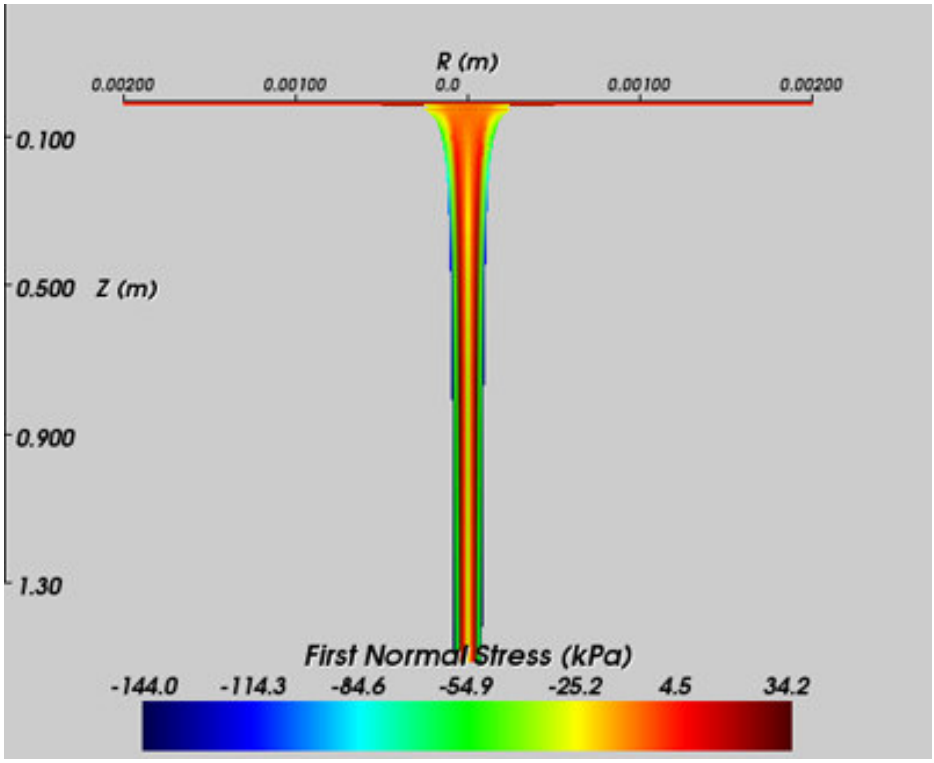


Figure 3.2 2D plot of the stress level of the polymer. Image created in VTK. [CAEF06]

3.1.3 OCTA Project

OCTA, which means “growth for future” in Japanese, is an integrated simulation system used to visualize the continuum level of polymer materials [OCTA06]. This system, led by Professor Doi, focuses on soft materials such as colloids, surfactants, and gels. OCTA is able to generate the equilibrium molecular configuration for a given density profile of atoms. In addition, it is able to calculate the rheological properties of polymeric liquids

based on the molecular weight distribution and branching structure. Figure 3.3 displays one type of output created by OCTA.

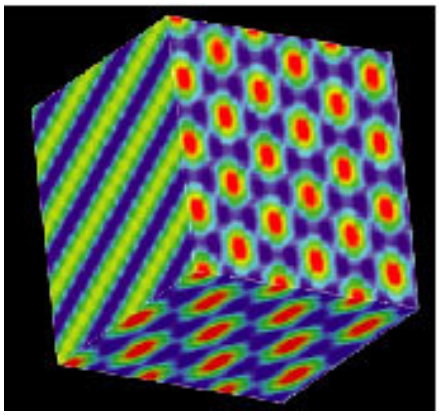


Figure 3.3 Self-organized structure of block copolymer in OCTA [OCTA06]

3.1.4 ParaView

Another visualization system used to visualize large sets of data is ParaView. This open-source, multi-platform visualization application provides filters by default such as extraction, reflection, extrusion, and smoothing on primitives [PARA06]. Users are also able to change the parameters of many filters by interacting with the 3D view and maintain interactive frame rates during large data models. Since all filters produce datasets, users can save the result of every operation as a data file. In addition, glyphs such as arrows, cones, lines, spheres, and various 2D glyphs can be applied to the points in a dataset. These glyphs can be scaled by scalars, vector component or vector magnitude. Figure 3.4 shows a snapshot of the capabilities of ParaView.

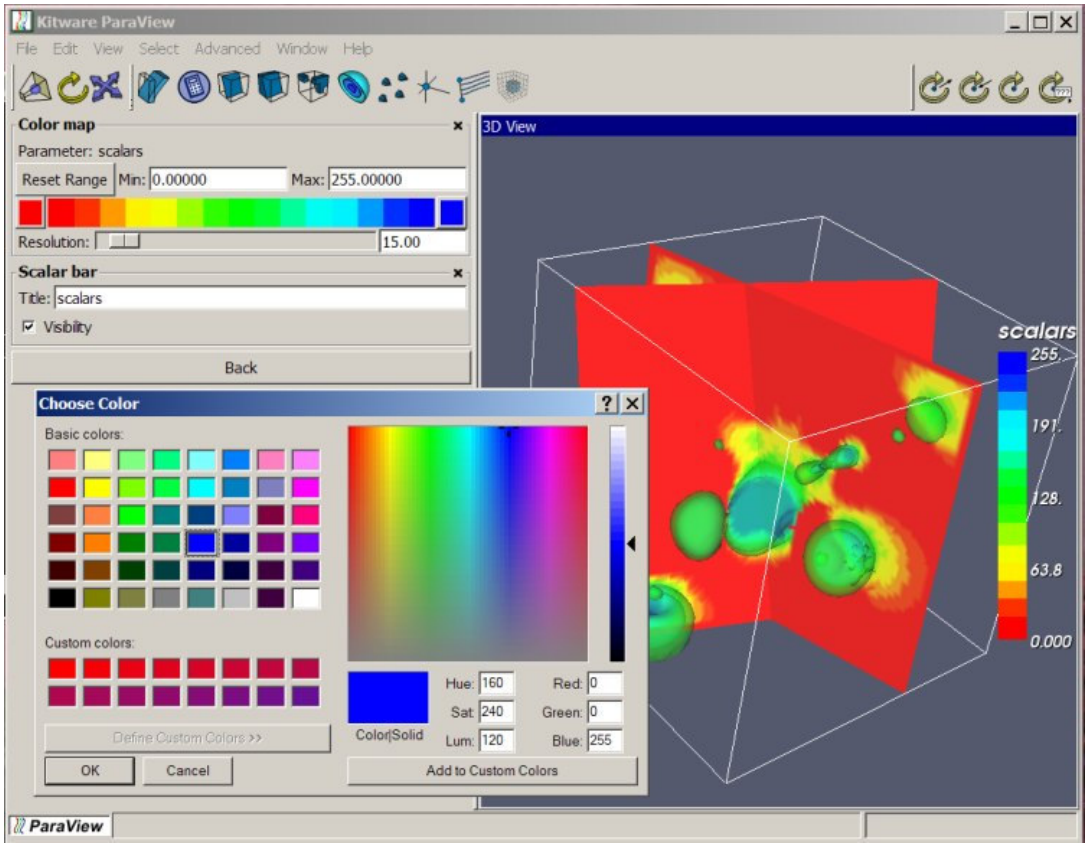


Figure 3.4 High potential wave function values around an iron protein molecule [PARA06]

3.1.5 MOLEKEL

MOLEKEL is an interactive, 3D molecular graphics software used to visualize data from a variety of electronic structure program outputs [MOLE06]. This application can render transparent objects, can overlay molecules on top of each other, and has animation capabilities. A technique MOLEKEL uses to texture map surfaces is to color code objects based on the molecular electrostatic potential. The software also represents molecules as wire frame, stick, ball-and-stick, and spacefill representations, as shown in Figure 3.5.

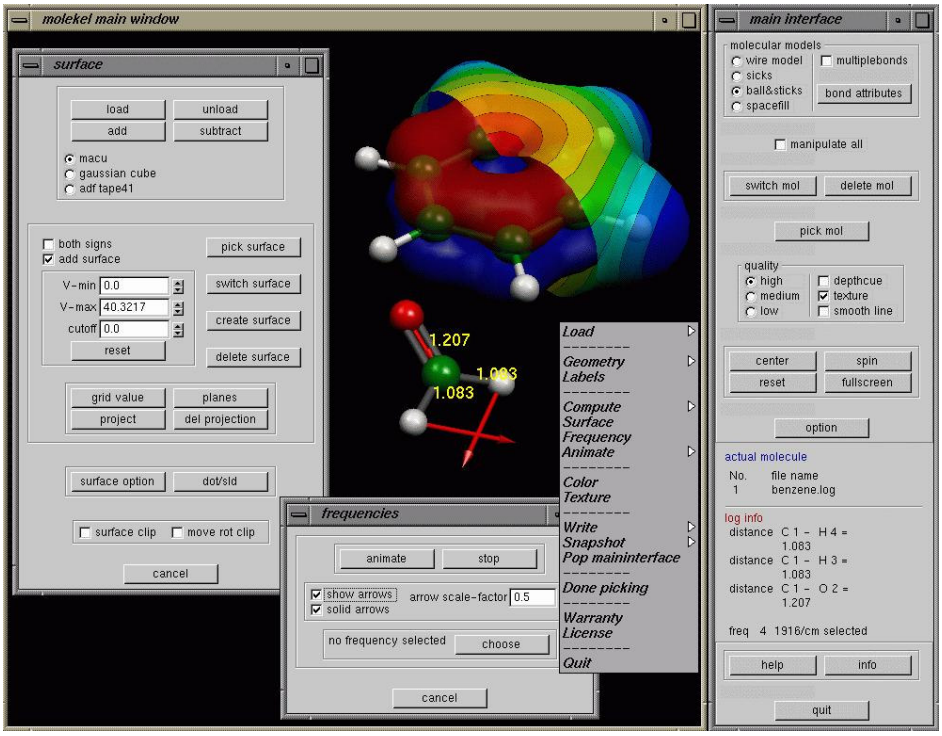


Figure 3.5 MOLEKEL consists of a main graphics window and several popup windows [MOLE06]

3.1.6 VuChem

VUChem, an advanced version of the scientific visual package VU, is a graphics software system that focuses on the visualization of molecules and analysis of mathematical data [IV06]. The system displays geometry as NURBS surfaces. Users also have interactive control of the animation and are able to save the animation as an mpeg file. VUChem allows particles to be displayed as lines/tubes and spheres, with the size of the particle controlled by variables or expressions. Figure 3.6 displays an output image from VUChem.

In the next section, we discuss these current tools and their limitations.

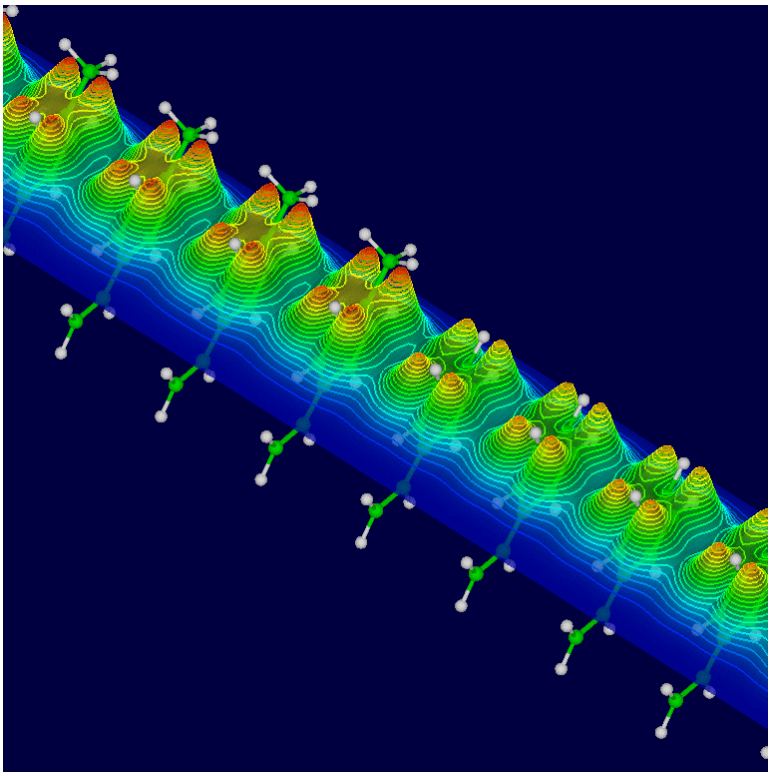


Figure 3.6 Output image in VUChem [IV06]

3.2 Discussion of Current Tools

We desire to use Maya's high-end graphics for our animation. Since visualization packages are created to be interactive, less emphasis is placed on the artistic nature of the software. Thus, the render outputs from these visualization tools are not as compelling as the images produced in Maya. However, animations created in Maya do lack some interactivity, which is one of Maya's disadvantages. Nonetheless, other limitations found in these visualization packages make Maya suitable for our application. For example, even though VTK has great imaging and visualization capabilities, it is not a fast graphics engine [VT06]. Thus, if we desired to create a quick particle system, it would be best to use a high-end 3D graphic software such as Maya to perform the simulation because of its playback capabilities.

Within the OCTA environment, the properties of polymers are determined by material characteristics such as molecular weight, molecular weight distribution, branching structure, degree of chain orientation, degree of crystallization, and the states of the crystal-amorphous interfaces. Thus, building a single simulation system of polymer materials is not easy. The dilemma becomes even more complicated in the case of polymer blends or composites where the dispersion state and the interfaces between the component phases alter the material property drastically. Thus, the morphology of polymers presents a challenge for OCTA. In addition, the software does not create any animations of fiber and film processing. Development of such an animation that focuses on the fiber and film process at the continuum level would enhance the way students, researchers, and industrial workers learn about polymers by adding a more realistic, yet at the same time artistic perspective.

Although ParaView's main strength is its ability to interactively view very large datasets, its main weakness is its inability to handle transparent surfaces [TERA06]. In contrast, Maya, which handles transparent primitives, gives us the capability in controlling the level of opaqueness on our glyphs as they float inside the polymer. Since we may desire to distinguish which particles are being crystallized, this feature in Maya will allow us to show a contrast between these particles.

Since MOLEKEL has limitations on how to represent data, such as representing molecules as wire frame, spacefill, and ball-and-stick, we prefer to create our animation in Maya. By using a particle system combined with bump map texturing, lighting, and other features in Maya, we can represent more information about the polymer. Thus, our imagination is not limited to the way we demonstrate this molecular process.

VUChem lacks texture mapping, which makes Maya more suitable to use, as we can emphasize certain properties such as crystallinity through texturing. This feature allows us to effectively illustrate the relationship of dynamic quantities in our animation and the ability to create compelling imagery. In addition, VUChem limits the way we represent our particles. Since we desire to instance these particles with arbitrary shape or form, Maya allows us to create the preferred primitive and animate the geometry throughout the animation.

Now that we have discussed these software packages and their limitations, we explore another method used to represent molecular data in the following section.

3.3 Abstract Visual Animation

Although the focus in this animation is to create a realistic visualization of the continuum level of polymers, our secondary objective is entirely aesthetic. Thus, we desire to capture the beauty of scientific data as it represents certain phenomena found in nature. By highlighting certain visual elements such as lines, color, shape, rhythm, and movement in our animation, we are able to stimulate an emotional experience in the viewer.

Lane Last felt the beauty inherent in an image could cling to the imagination of a viewer without their knowledge of the specific information [HYLE06]. He believed appealing visual elements of an artwork could ultimately become an opportunity to educate in an informal fashion. Last's repetition of cool and warm colors, shapes, and lines add a sense of contrast and harmony in his version of electronegativity in Figure 3.7. The structure of molecules attracting other electrons through covalent bonding

causes the viewer's imagination to focus on the aesthetic behavior of atoms rather than how these bonds actually occur in nature. Last believed creating an abstract art piece challenges the imagination of viewers to further their knowledge in the sciences, which is one of our primary goals.

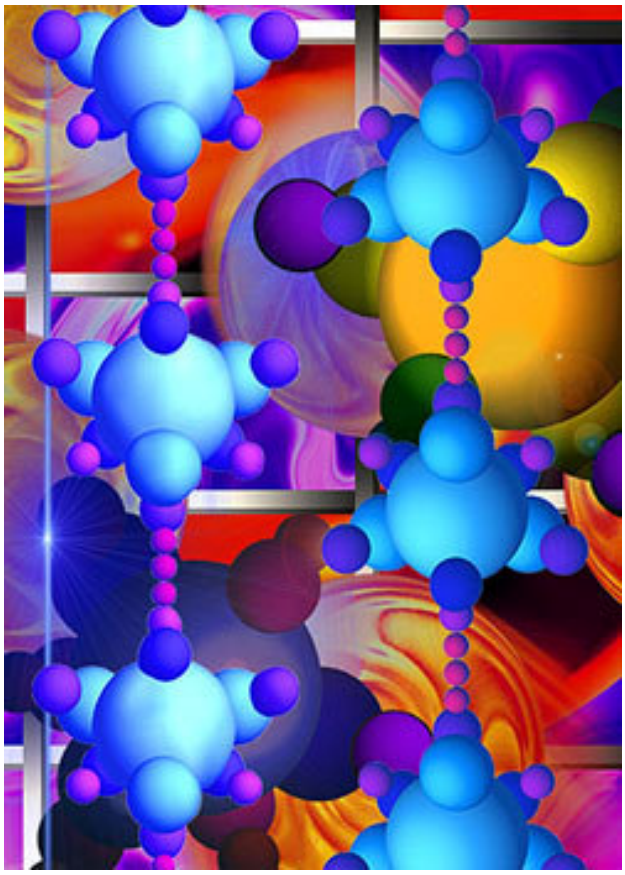


Figure 3.7 Abstract Image of Electronegativity by Lane Last [HYLE06]

Using abstract shapes and color, Richard Gillilan is able to produce an interesting image of two immune system proteins joining together, as shown in Figure 3.8 [MGL06]. His repetition of shapes floating in air causes movement and depth of field within the artwork. Although very difficult to understand, Gillilan's use of dark colors expresses a sense of mystery in the scene. As a result, he manages to express his uncertainty about the environment surrounding the proteins, while creating an emotional response.

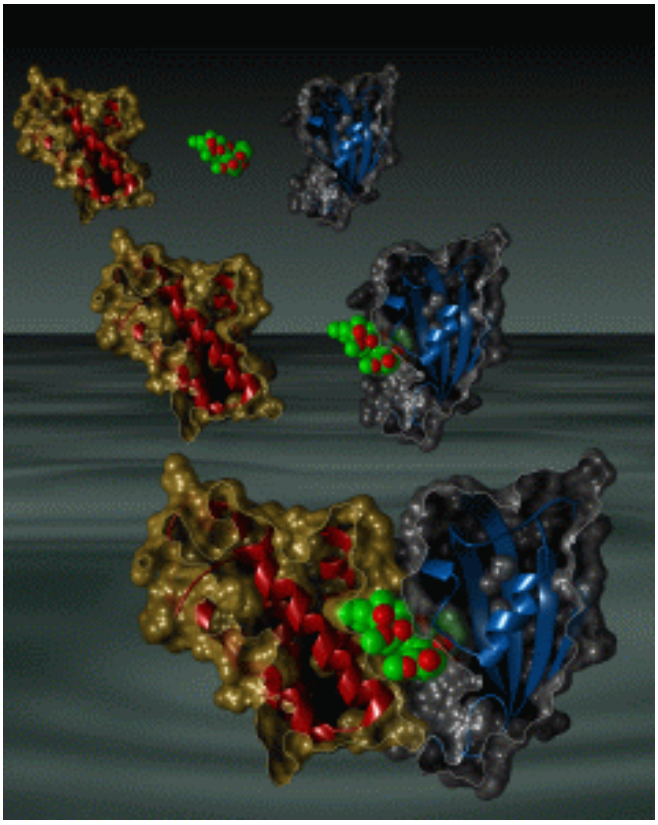


Figure 3.8 Abstract image of proteins by Richard Gillilan [MGL06]

In his thesis entitled, “Interpreting Data: From Scientific Visualization to Visual Abstraction,” Marc Bryant produces a visual abstraction of a polyethylene molecule undergoing crystallization, as shown in Figure 3.9. Bryant’s use of the “ribbon” method to display the crystallized backbones of the molecules was effective, as it captured the tension inherent in the configuration changes of the polymer [BRYA03]. Through abstract shapes, lighting, shading, and music, Bryant was able to create mood and emotion in the scene. Although based upon scientific data, his animation of crystallinity is an artistic experiment in visual interpretation. In the next section, we discuss the artistic decisions of these abstract works.

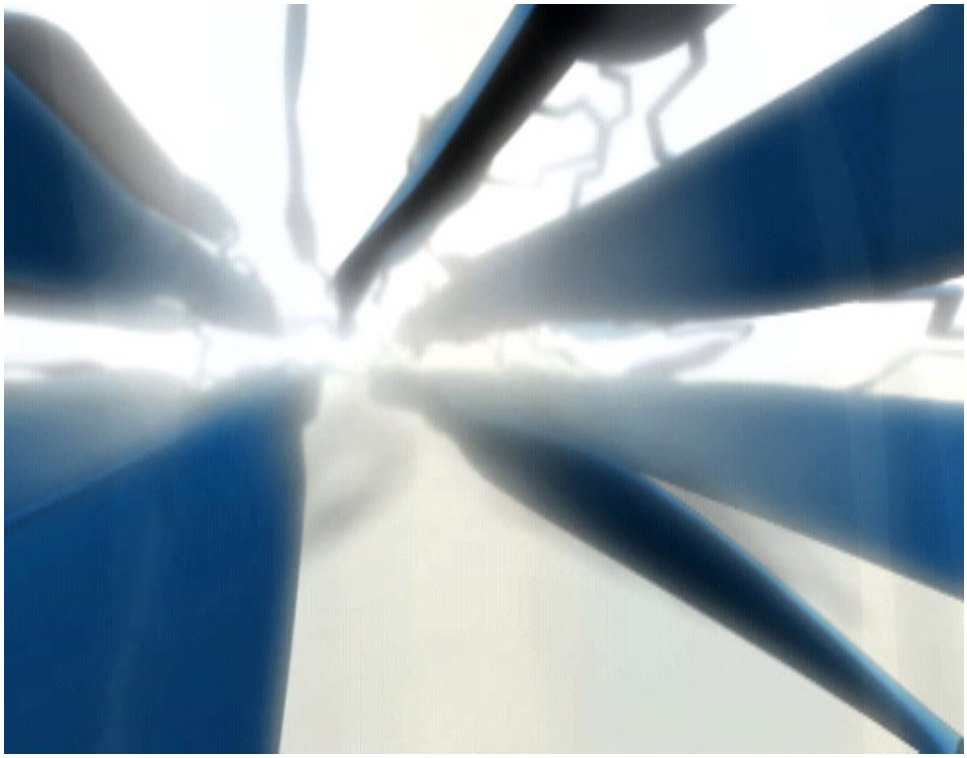


Figure 3.9 Marc Bryant's image of a polyethylene undergoing crystallization [BRYA03]

3.4 Artistic Discussion

Although Lane Last and Richard Gillilan create abstract images of different molecular processes, texturing would add more contrast and distinction to these visuals. In addition, an animation of both processes would be more effective than a still image, as this adds motion and rhythm to the scene. Even though Marc Bryant's animation captures these principles of design, it does lack texturing. Our decision to use textures to illustrate crystallinty gives more variety and emphasis to our animation.

In the next chapter, we discuss our implementation and artistic decisions.

CHAPTER 4

IMPLEMENTATION

This chapter outlines our solution to producing a realistic representation of the continuum level process via animation. We wish to create a particle system flowing inside of a polymer, as this system displays certain dynamic quantities. Since there was no preference in the type of polymer to be visualized, one was randomly chosen for this animation. Section 4.1 discusses the method used in illustrating temperature, velocity, crystallinity, and tensile stress. In Section 4.2, we demonstrate how our techniques contribute to our secondary objective of creating an aesthetic illustration of this phenomenon.

4.1 Methodology

We approach the problem of polymer visualization by first obtaining 2D modeling results of the continuum level from FISIM, a software package created by CAEFF. The FISIM software, which stands for Fiber and Film Simulation, is capable of predicting final properties for a given polymeric material in an industrial fiber and film process. With these results, a visual representation of certain dynamic quantities such as temperature, velocity, crystallinity, and tensile stress of a particular polymer is achieved.

The first dynamic quantity we desired to visualize was temperature. As shown in Figure 4.1, cooling occurs on the exterior portion of the polymer while the interior part remains the hottest. To represent this property, multiple emitters releasing different

colored particles were used. In addition, we desire the particles to flow in a die swell shape. Since the actual shape of a polymer generated by the FISIM model had already been acquired, the particles simply needed to flow along the surface. Using goals for Maya particles accomplished this task. A goal is an object that particles flow or move towards, in this case, the die swell object. Goal weight sets how the particles of the emitting object are attracted to the goal. A value of 0 means that the goal's position has no effect on the trailing particles, while a value of 1 moves the trailing particles to the goal object position immediately. Since the particles should flow along the surface, a goal weight of 1 was appropriate. However, to have the particles flow from the top of the surface to the bottom, two dynamic attributes were added to the Per Particle (Array) Attributes – goalU and goalV. These attributes, which are found in the General Tab below the Add Dynamic Attributes Tab located under the particleShape's Tab of the particle, allows particles to flow in the horizontal and the vertical directions, respectively. Since the particle's lifespan is based on its horizontal or U position, a ramp was used for the goalU's parameter. In Figure 4.2, white means birth and black means death. By adjusting the ramp to these colors, the particles are born at the top of the object and die at the bottom of the surface. The particles also needed to begin at random positions as they flow in the V direction. For goalV's parameter, the expression, particleShape1.goalV = rand(0,1), was used to produce the effect shown in Figure 4.3.

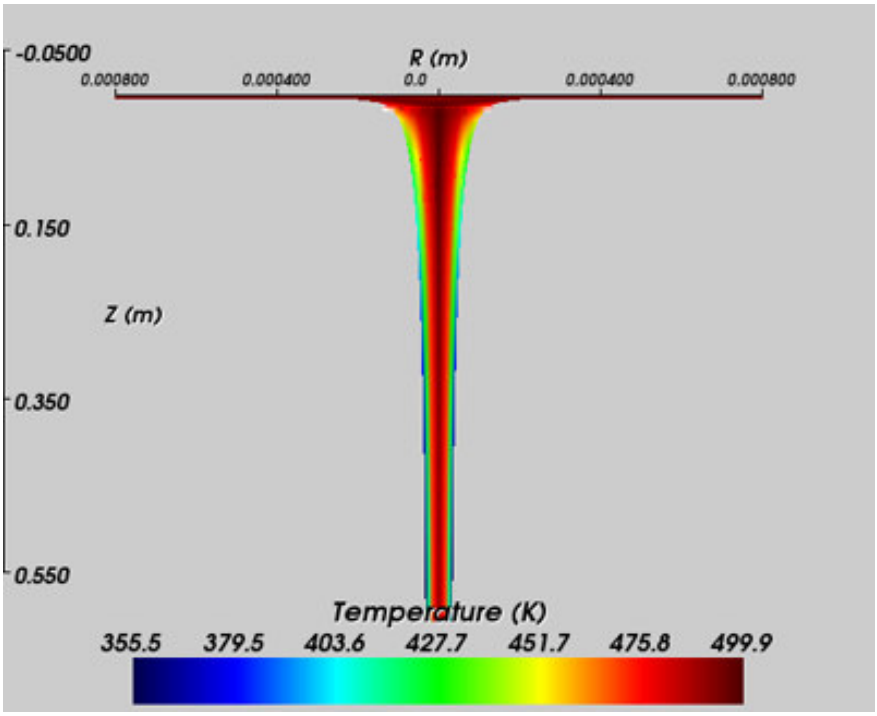


Figure 4.1 Temperature of a particular polymer taken from FISIM Model [CAEF06]

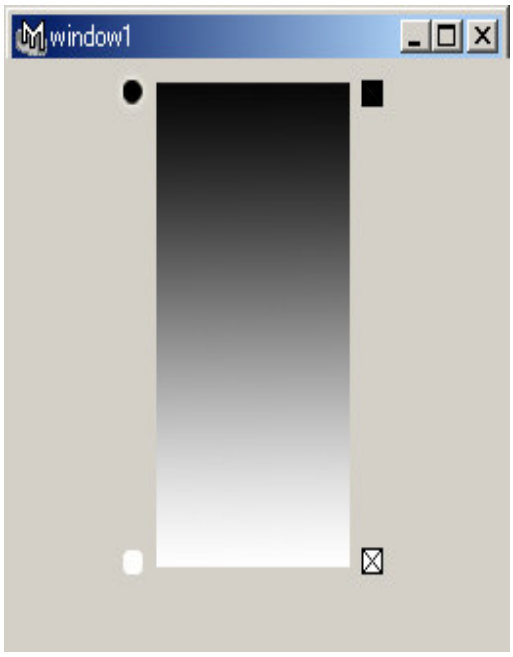


Figure 4.2 Ramp used for goalU's parameter

Figure 4.3 Particles flowing in the vertical direction.

Since it is cooler on the exterior of the polymer than in the interior part, we still needed to show a variation in color. Our first idea was to place different emitters inside the die swell and change the color of each particle. However, we noticed the particles inside did not flow as smoothly as the particles did in Figure 4.3. Thus, we decided to create three die swells inside of the first one and repeat the same technique of using goals. These multiple swells would be hidden in the scene to make it seem as though particles were flowing inside of the original die swell. Figure 4.4 shows a top view of this method. It should be noted that each color shown in the figure represents a different position of the multiple die swells and each particle's color. In addition, the inner particles would have a glow effect to show the intensity of the heat inside of the polymer. This was an effective technique as it allowed us to have better control of the flow of particles and to show the variation in temperature.

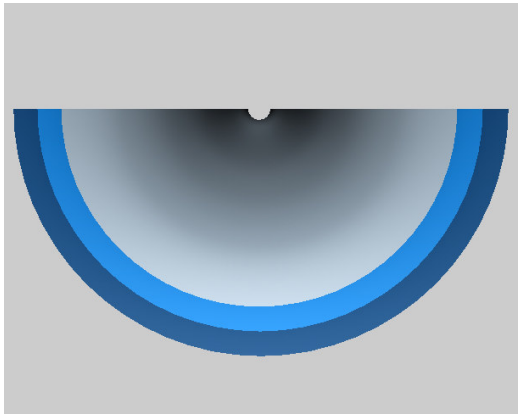


Figure 4.4 Top view of different die swells

The next dynamic quantity visualized was velocity. As shown in Figure 4.5, after exiting the die, the polymer comes out slowly but gradually increases in speed. Thus, we needed to adjust the flow of particles in the model. Since the particles are attracted to the goals in the scene, we discovered we could use the Lifespan Mode to determine the speed

of the particles. This attribute is found under the particleShape1 Tab of the particles and provides four options to choose from: live forever, constant, random range, and lifespanPP only. Since the live forever option means the particles will never die, the ramp set for goalU's parameter will not be effective because the particles are set to die at a given U or horizontal position. The constant option allows the user to determine how long it takes for the particles to reach their destination points. Thus, the higher the number specified, the slower the particles move to reach their goals. This option does not satisfy our solution since the particles need to gradually increase in speed. The Random range option also sets the speed of the particles to a random constant number. Since this option will not accomplish our goal, we decided to use the lifespanPP option. This tool allows the user to write an expression for each particle's lifespan. However, the dilemma was specifying the initial speed of each particle before gradually increasing it over time. Since each particle started at the top of the die swell, its Y position would be higher than at the bottom of the die swell. If the lifespan of the particle is set to the particle's initial Y position, the lifespan will decrease once the particle reaches its goal. Thus, this decline will accomplish our goal of gradually increasing each particle's velocity. After selecting the lifespanPP option, we created the following runtime expression for the lifespanPP attribute listed under the Per Particle (Array) Attributes Tab:

```
vector $pos = particleShape1.position;
particleShape1.lifespanPP = $pos.y;
```

This expression was written for each particle and its corresponding goal in the scene.

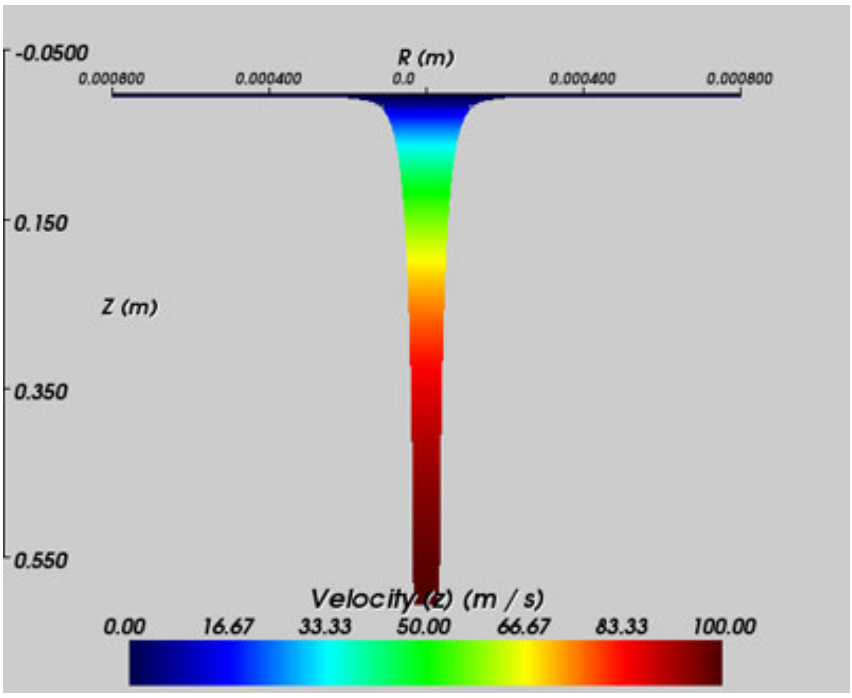


Figure 4.5 Velocity of a particular polymer taken from FISIM Model [CAEF06].

Crystallinity was the next dynamic quantity visualized in the model. As shown in Figure 4.6, crystallinity occurs near or on the exterior portion of the polymer. We also noticed that the percent crystallinity increases over time. Our objective here is to create a contrast between non-crystallized and crystallized layers. To illustrate this distinction, we decided to create an animated bump map texture on the particles that were experiencing this phenomenon. In Maya, bump maps are grayscale textures mapped to objects to create the illusion of surface relief on an otherwise flat object.

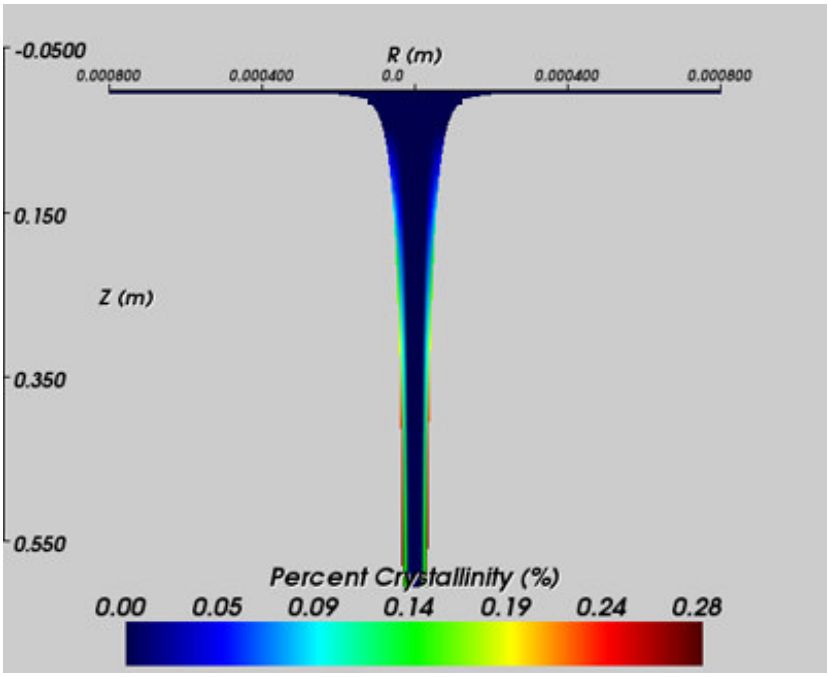


Figure 4.6 Crystallinity of a polymer taken from FISIM model [CAEF06]

The first step in this procedure is to map a Blinn material to each particle to produce a shiny surface. We also selected a texture to be used as a bump map for the material. We decided to place a Noise texture on the particle's surface because of the interesting fractal bumps it displays. Also, to create a more abstract representation of crystallinity, we adjusted some of the parameters under the Noise Attributes Tab.

The option that created an interesting effect was the Amplitude parameter. This parameter allowed us to adjust the depth of bumps on the particles. Therefore, we keyframed this attribute to give the illusion of crystallites growing over time. Figure 4.7 illustrates a particle's surface after a noise texture is applied as a bump map.

(a) (b) (c)

Figure 4.7 (a) Particle surface after 1 second. (b) Particle after 3 seconds (c) Particle after 6 seconds

Before validating this representation, we found an interesting picture of the growth of crystallites, shown in Figure 4.8. Note how the squares grow over time, but not necessarily in dimension. This figure could be compared to a sea of fish in an ocean. Sometimes, to protect themselves from predators, fish align adjacent to each other to appear as one huge fish. From analyzing this figure, we concluded the noise texture application did not give us an accurate representation, as it illustrated the bumps gradually enlarging over time rather than growing in an adjacent fashion.

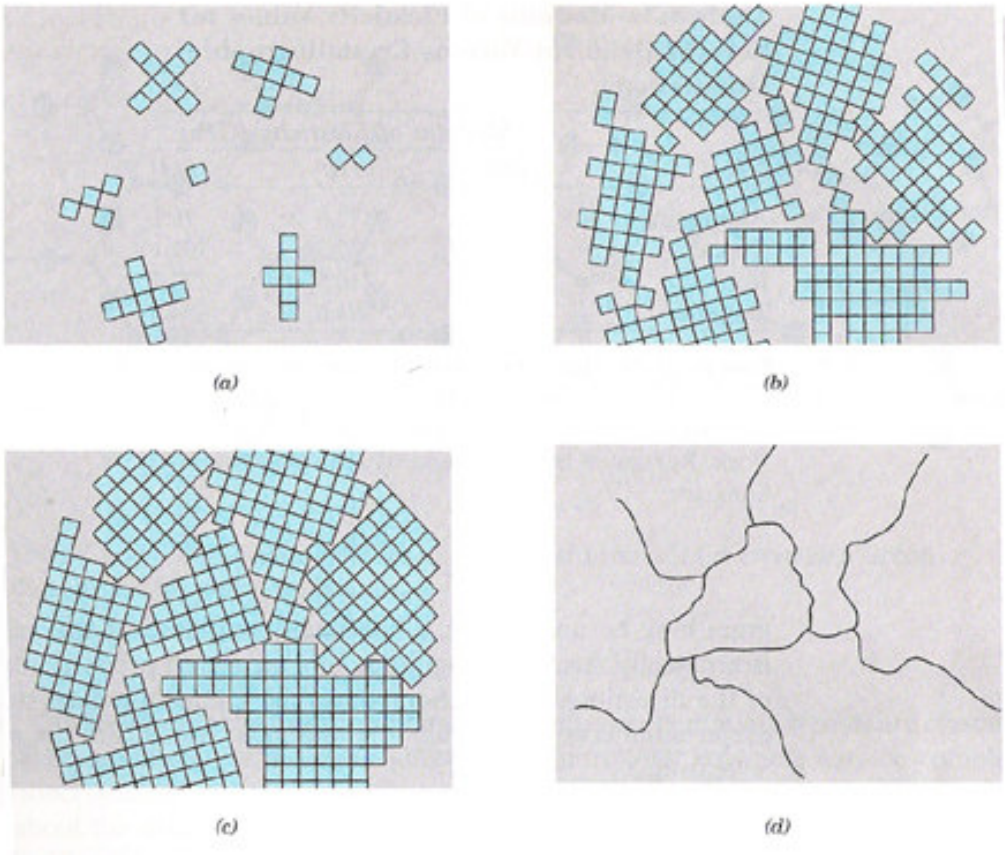


Figure 4.8 (a) small crystallite nuclei (b) growth of the crystallites (c) irregular shapes have formed (d) dark lines representing the grain boundaries as it would appear under the microscope [CALL03]

To illustrate the growth of crystallites, we decided to create a sequence of images in Adobe Photoshop and map it to the surface of the particle. Even though this process is tedious, it allows us to control how these crystallites grow on the surface. However, before creating the sequence, we needed a source image that represents crystallinity. After discussing this subject matter with polymer scientists and engineers, it was determined that crystallites could be represented as tiny snowflakes growing on the surface. Figure 4.9 illustrates the snowflake image we decided to map to the particles.

Figure 4.9 Snowflake image used to represent a crystallite structure [CLAS06]

In Photoshop, we created twenty-four distinct images of multiple snowflakes adjacent to one another and changed the opacity value on some of the snowflakes. The reason for altering the opacity value was to give the illusion that the snowflakes were gradually appearing on the surface over time. Figure 4.10 illustrates an image with multiple snowflakes. In addition, since we wanted the sequence of images to last for twenty seconds, we made twenty copies of each image. This produced a total of 480 images.

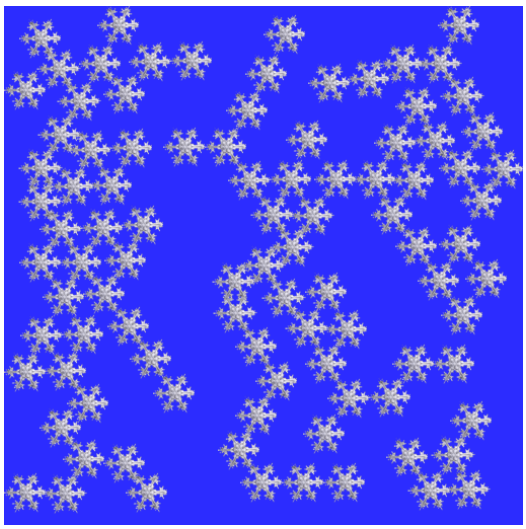


Figure 4.10 Snowflakes placed adjacent to one another

After creating the sequence of images, we imported them into Maya. Instead of choosing the Noise Material this time, we selected the File Texture button. The File Texture node allows bitmaps scanned from photographs, taken with a digital camera, or painted in a 2D or 3D paint program, to be transferred into Maya as a bitmap. We used the Use Image Sequence option under the Image Name Tab to load the sequences into Maya. The image sequence used as a Bump Map Texture created the illusion that the surfaces of the particless were changing due to crystallinity. Figure 4.11 illustrates a particle with the File Texture node applied to it.

(a) (b)

Figure 4.11 (a) Particle's surface after one second (b) Particle's surface after 15 seconds

The final quantity visualized was tensile stress. As shown in Figure 4.12, high tensile stress can occur in the interior of a polymer. However, it should be noted that high tensile stress can occur in any location, depending on the stress applied to the polymer.

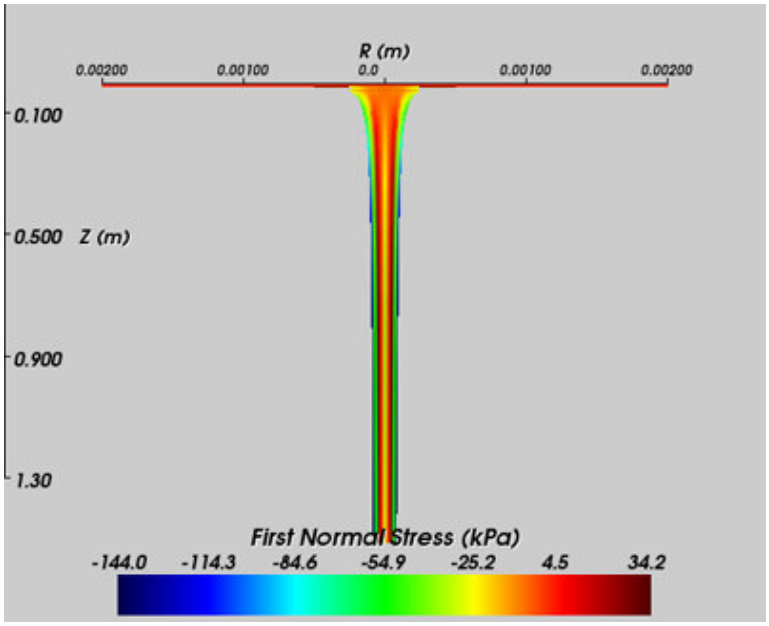
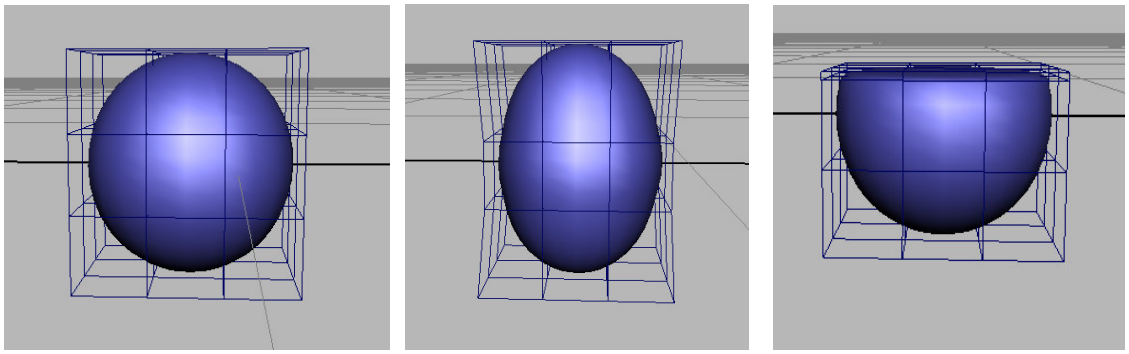


Figure 4.12 Tensile stress of a polymer taken from the FISIM Model [CAEF06]

Since tensile stress deals with a polymer elongation over a period of time, we can represent this quantity by stretching a sphere into an ellipsoid over time if the value is positive, or into a collapsed shape if the value is negative. To have more control in the stretching of the object, we inserted a lattice deformer around the sphere to alter its shape, as shown in Figure 4.13. In Maya, a lattice is a structure of points carrying out free-form deformations on any deformable object. Thus, by setting keyframes on the points of the lattice over time, we could create the desire shapes. Finally, after analyzing the variation of stress levels depicted in the graph, we instanced a sphere morphing into an ellipsoid onto particles that exhibited a positive tensile stress and instanced a sphere morphing into a collapsed shape onto particles that displayed a negative tensile stress.



(a) (b) (c)

Figure 4.13 (a) Sphere's surface before being stretched (b) Sphere stretched into ellipsoid after 8 seconds (c) Sphere collapsed after 8 seconds

4.2 Artistic Implementation

Now that we have visualized temperature, velocity, crystallinity, and tensile stress, we focus on the visual abstraction in the scene. To emphasize the temperature profile of the polymer, we disregard the traditional colors of blue and red to show cool and warm temperatures, respectively. By only using a palette of blue colors and adding a glow effect on the interior particles to illustrate heat, we create a more abstract, artistic representation of the variation of temperature throughout the polymer. In addition, visualizing the change in speed of the particles creates a more interesting animation. Typically, a visualization that is too uniform, such as having particles flow at the same speed, is not as compelling since there is no contrast in the animation. Since one of our goals is to bring the animation to life, variation in speed accomplishes this goal, as it adds tempo to the scene. Our intent is that this shift of motion captures the beauty of the molecular process and stimulates an emotional response in the viewer.

The use of textures in the animation produces a visual abstraction of the particle's surface as it experiences crystallinity. We are able to use this abstraction to manipulate the elements of art so the viewer is drawn to this particular part of the animation. Also, by

using different shapes to illustrate tensile stress, we add more variation and contrast to the scene, and thus create a more compelling and artistic animation. Even though the viewer may have no knowledge of the molecular structure of crystallization, we are able to produce a visual abstraction that illustrates contrast and growth. This abstraction allows the viewer to focus on the aesthetic nature of polymers and the scientific information being visualized.

We also decided a fly through animation inside the polymer would capture the very essence of molecular beauty. In order to accomplish this task, we open the mesh as it exits the dye and show the particles flowing inside. As these particles shift in speed, the viewer slowly journeys into the very heart of the polymer. It is in this place that the animation comes to life.

As the viewer travels through the polymer, the core of the polymer intensifies. This is where we desire to build an intimate connection between the viewer and the particles, as he or she explores the heart and soul of the polymer. Along the journey, we intentionally hide the inner particles and draw the viewer's attention to the exterior layer, which is experiencing crystallinity. This visual aid adds more emphasis, contrast, and beauty to the environment, as the viewer witnesses an unknown phenomenon. We then pull the viewer from this dreamlike world back into the macroscopic realm.

In the chapter that follows, we discuss the results from our implementation.

CHAPTER 5

RESULTS

In the fiber and film process, polymer chips are dropped into a hopper where they flow into an extruder to be melted. Next, the polymer travels through a filter and exits the die. As the polymer is flowing out of the die, it is wrapped around rollers.

The parts of the extruder model were assembled together to produce the picture shown in Figure 5.1. A blue background is placed behind the model to clearly indicate the design. In Figures 5.2 and 5.3, polymer chips are shown falling into the hopper and flowing into the extruder respectively. A polymer exiting the die is shown in Figure 5.4.

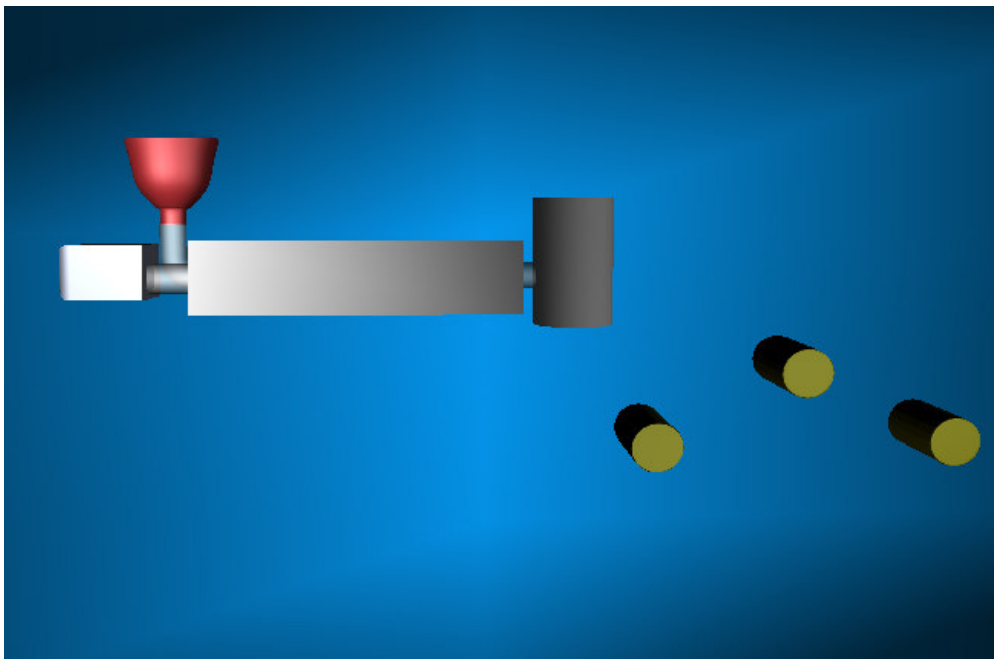


Figure 5.1 Extruder Model with a blue background

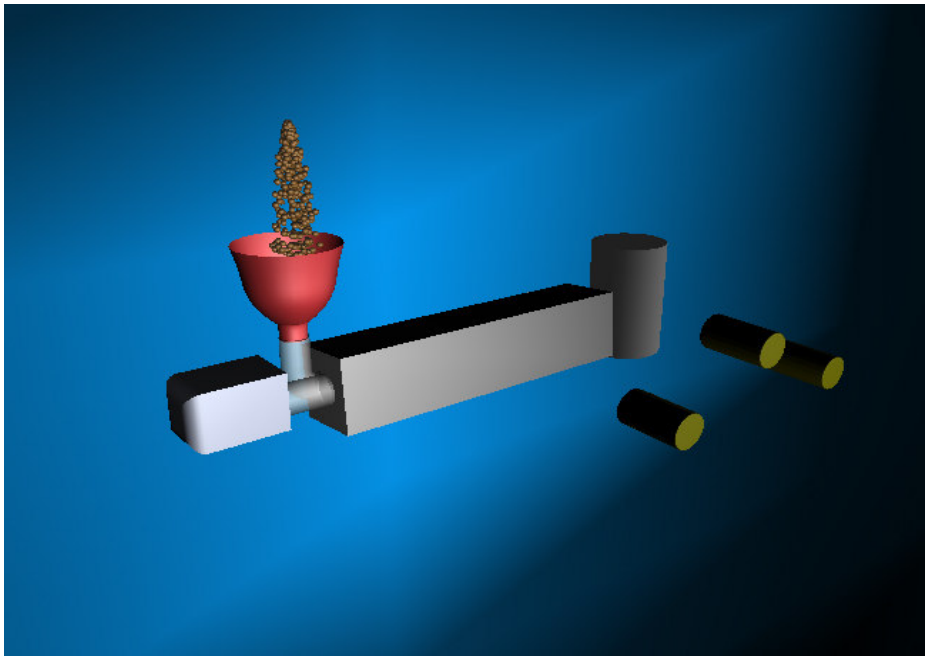


Figure 5.2 Polymer Chips falling into the hopper before being extruded

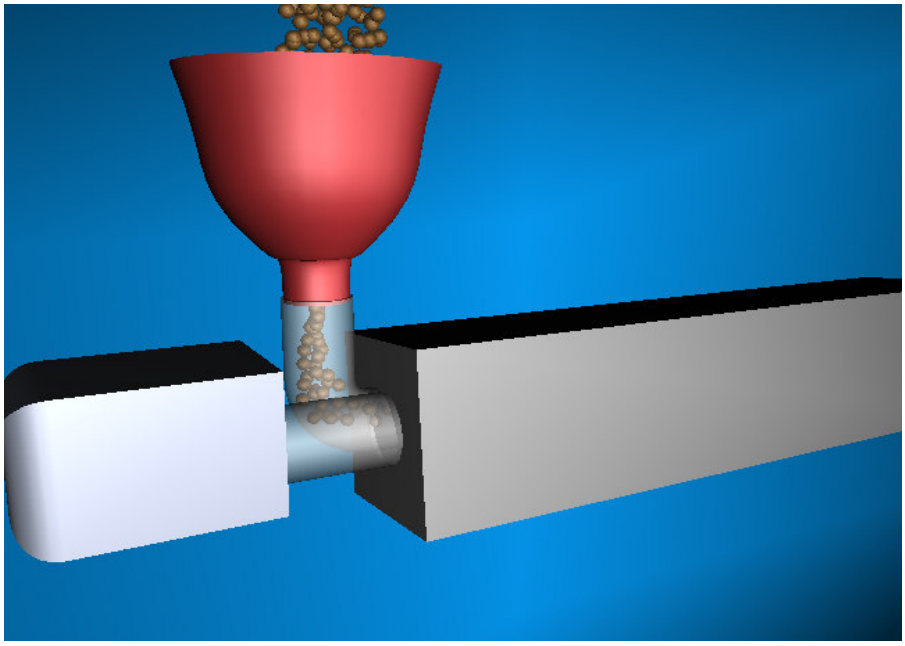


Figure 5.3 Chips flowing into the extruder

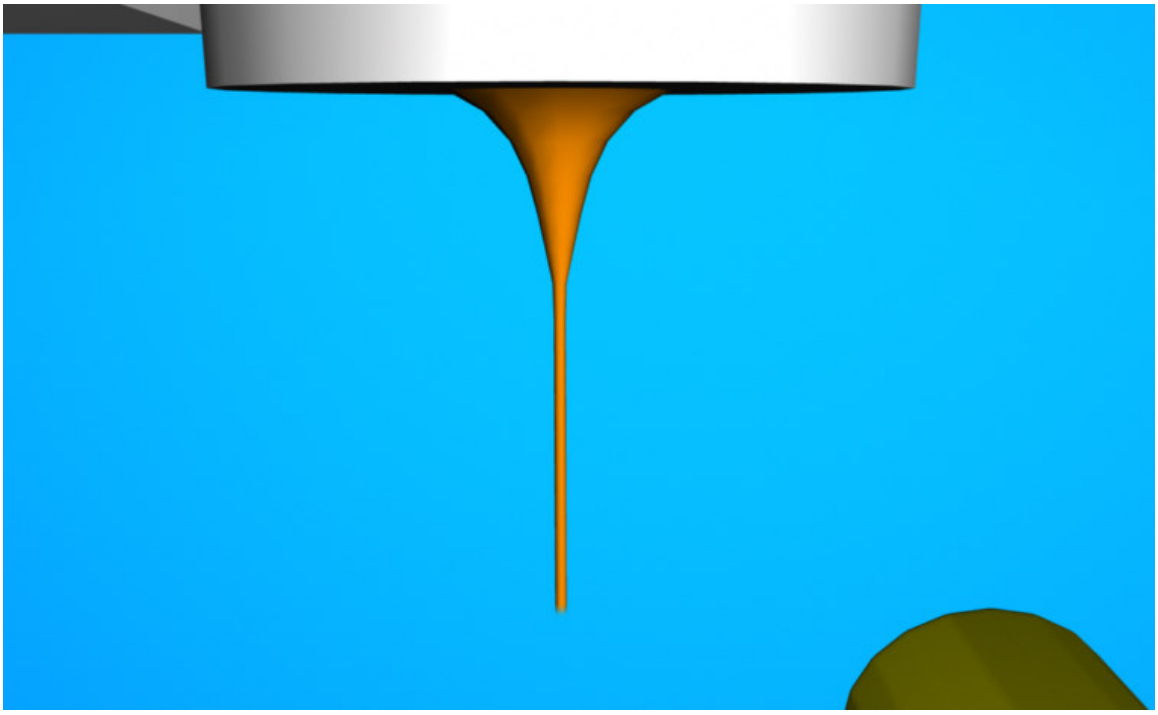


Figure 5.4 Polymer flowing out of the die

Next, the camera zooms into the polymer to focus on the macro level structure of the material. Figures 5.5 and 5.6 illustrate temperature change throughout the polymer, as the inner particles have a glow effect to reflect heat. Figures 5.7 and 5.8 demonstrate tensile stress by showing spheres changing into ellipsoids or collapsed spheres. Crystallinity is shown in Figures 5.9 and 5.10, occuring mostly on the exterior portion of the material. The animation concludes with the attachment of the die swell shape and an extruded surface wrapped around the rollers as shown in Figure 5.11.

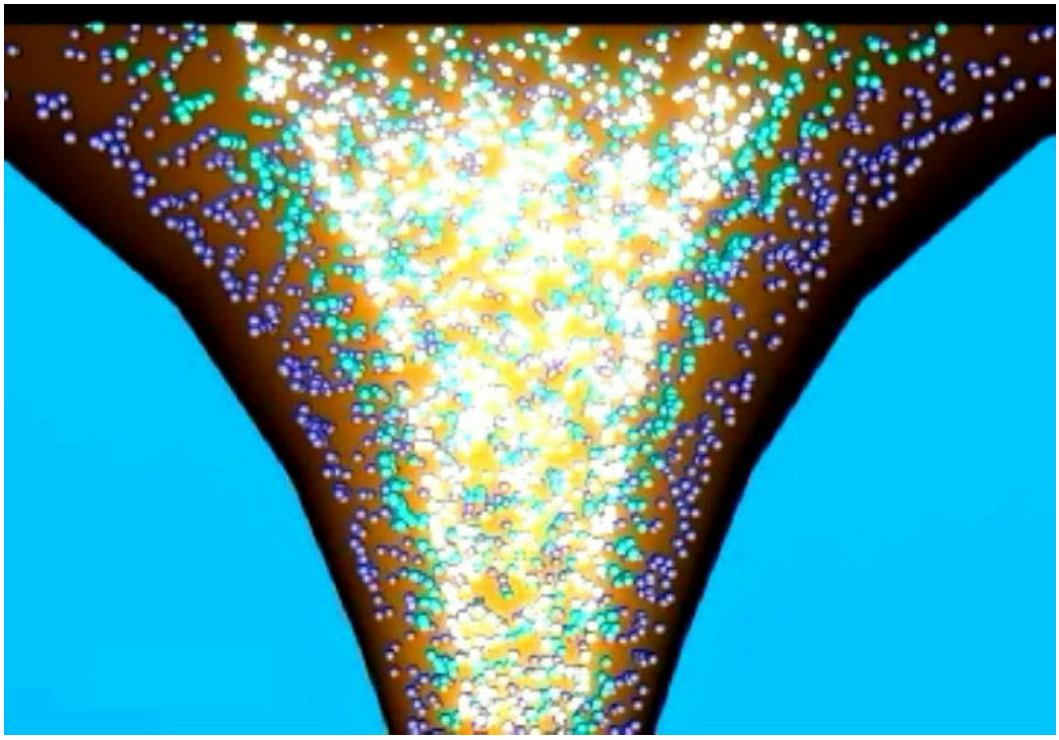


Figure 5.5 Inner particles (white) glowing to illustrate warm temperatures in the interior portion of the polymer. Simulation was performed at 24 framers per second (fps).

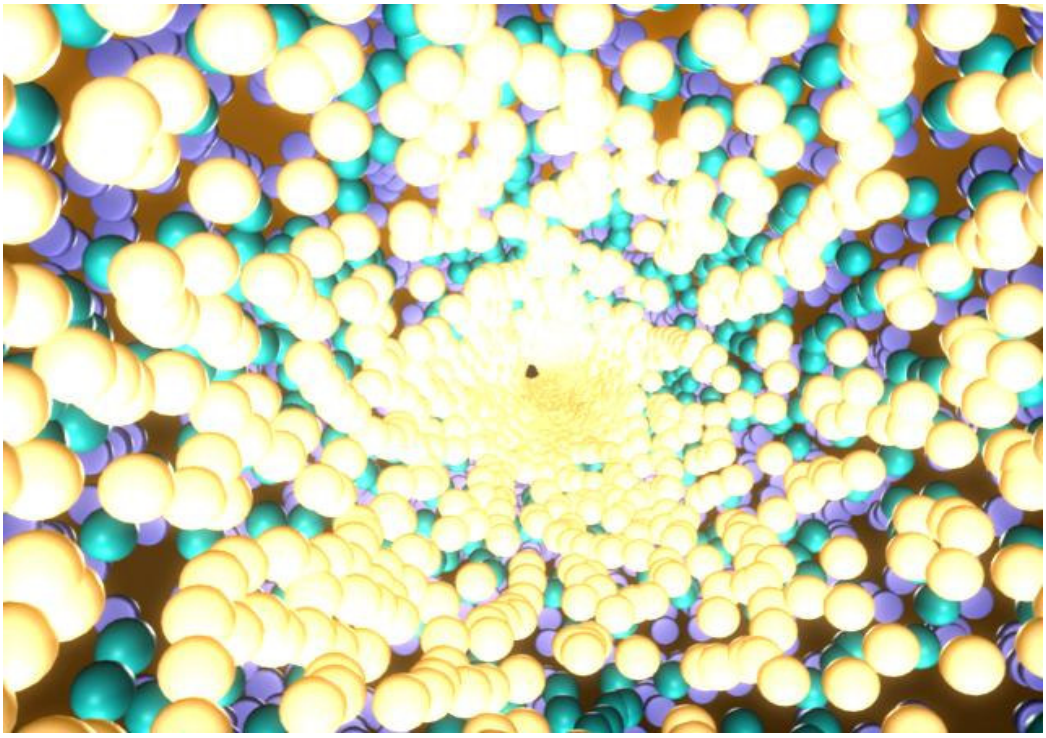


Figure 5.6 Closer view of temperature change after 15 seconds. Orange glow effect on white particles to illustrate heat. Simulation was performed at 24 fps.

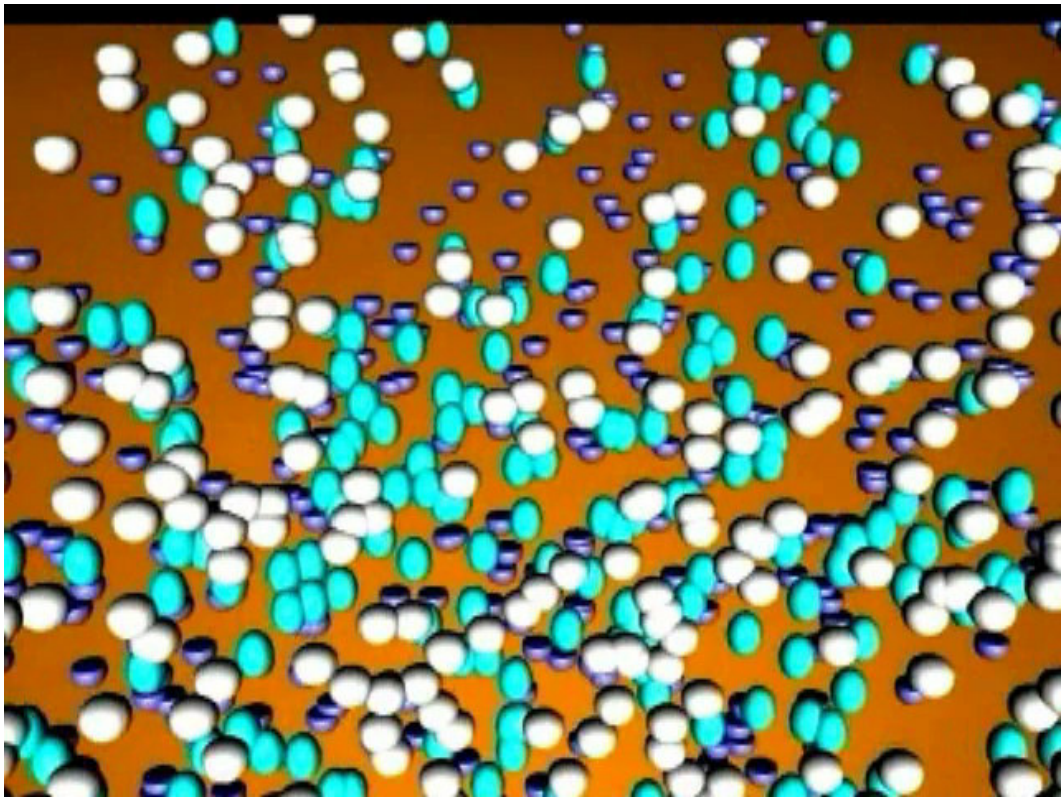


Figure 5.7 Tensile stress shown through ellipsoid and collapsed geometry. Simulation was performed at 24 fps.

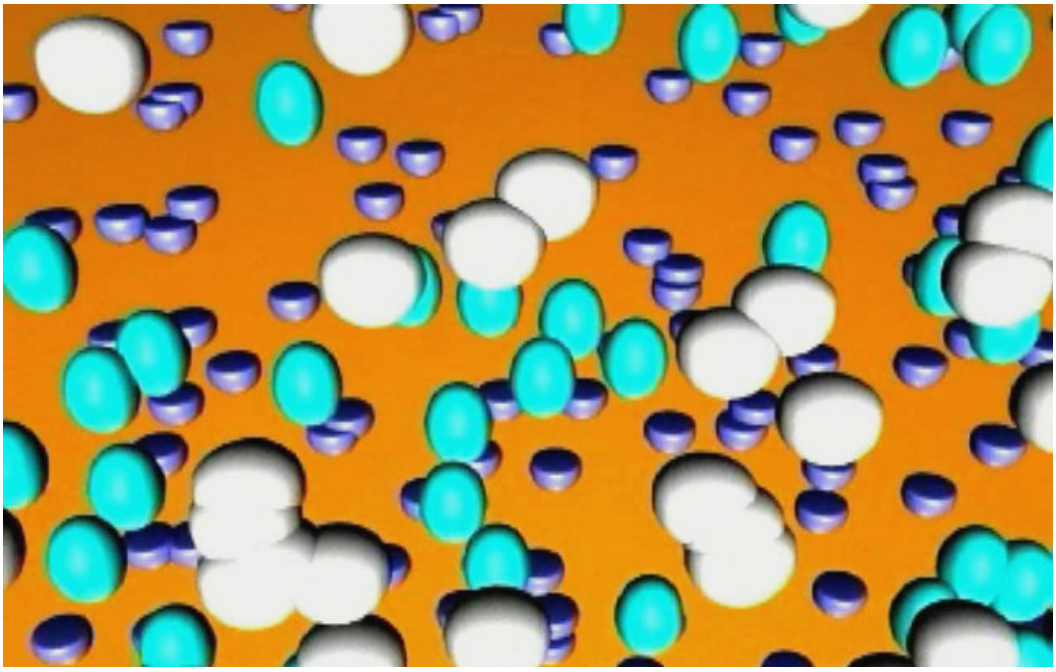


Figure 5.8 Closer look at the tensile stress illustrated with the ellipsoid and collapsed polygon. Simulation was performed at 24 fps.

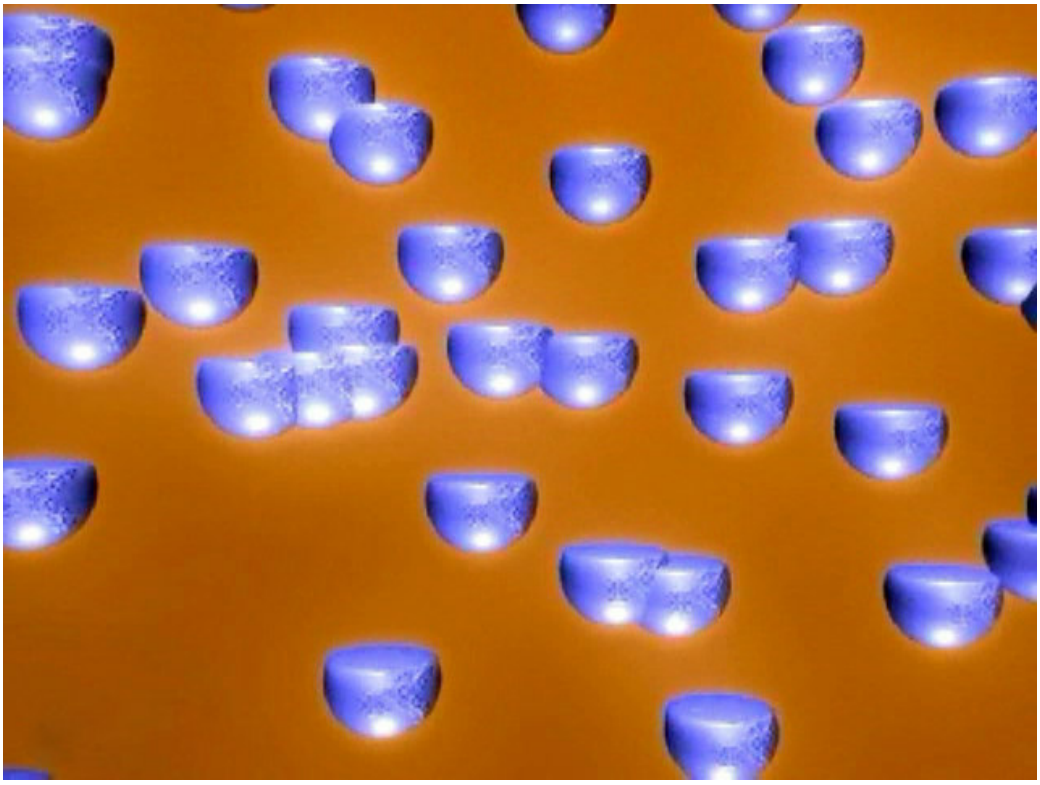


Figure 5.9 Crystallinity shown through the use of bump map textures along the surface.

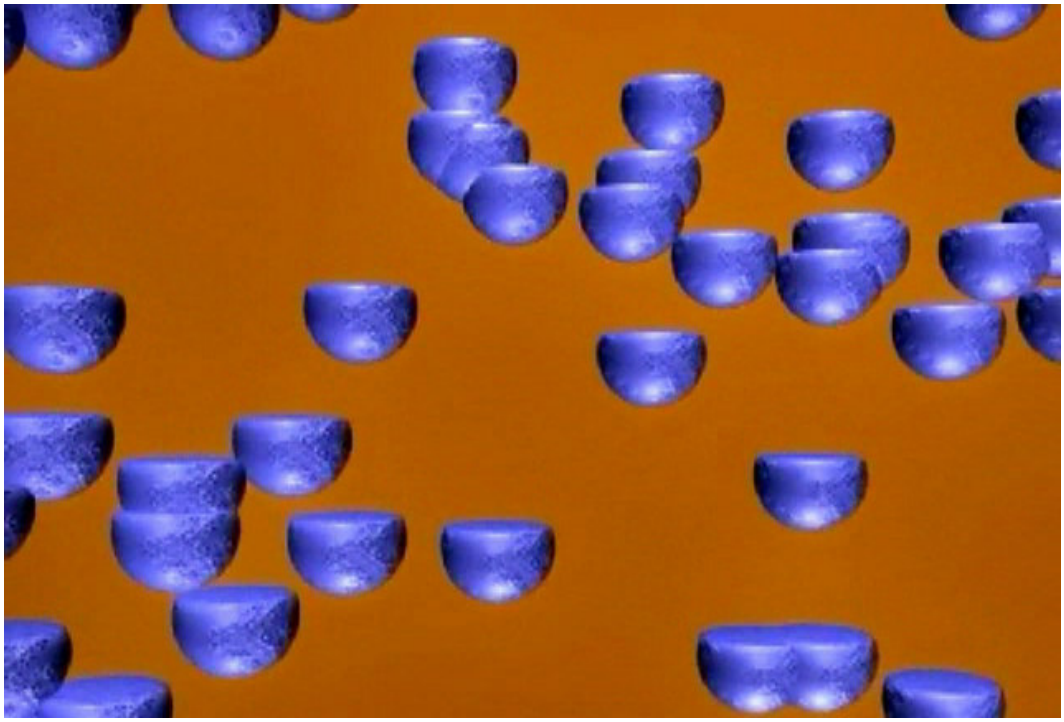


Figure 5.10 Polymer experiencing crystallinity on the exterior portion after 15 seconds. Simulation was processed at 24 fps.

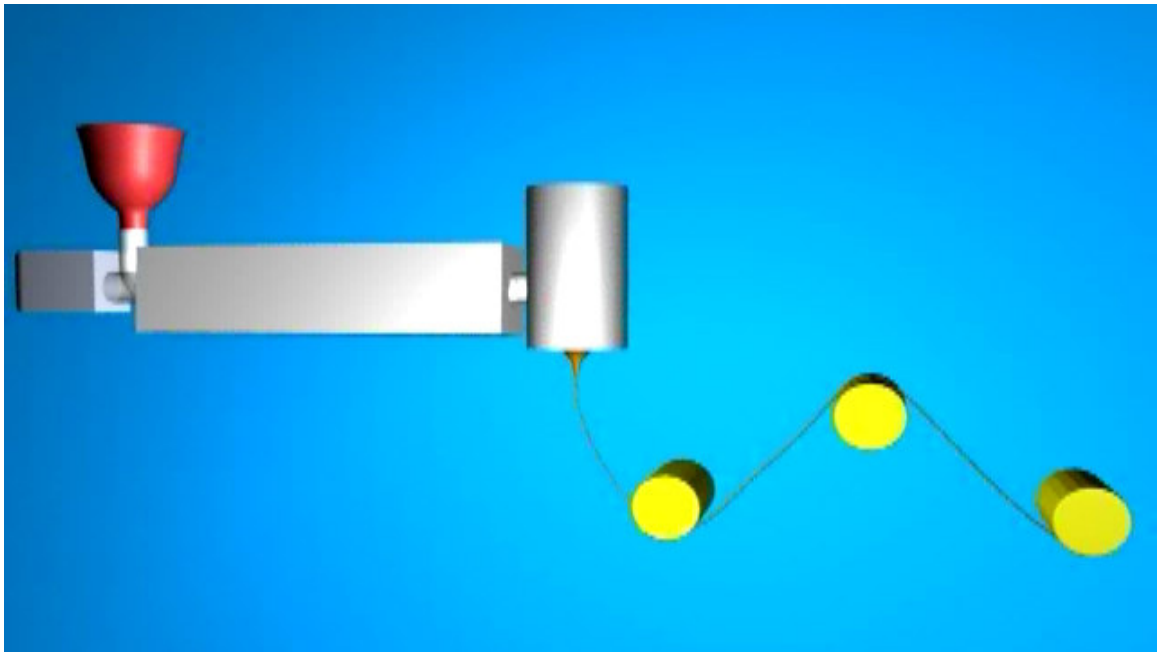


Figure 5.11 Polymer wrapped around rollers

The results of our animation give scientists a more in-depth knowledge about the relationship of dynamic quantities of polymers at the continuum level. In addition, our artistic decisions allowed us to present this information from a more abstract, artistic approach.

In the next chapter, we summarize the contributions of this work and possible future enhancements.

CHAPTER 6

CONCLUSION

Our goal was to create a more compelling scientific animation, as well as an abstract perspective, of the continuum level of polymer processing. Through this visualization, researchers will be able to better understand the properties of polymers and save time and money required for additional experiments. In addition, we illustrated the natural beauty of this molecular process through certain elements such as harmony, color, form, and texture. Visualizing other quantities such as orientation and tensile strength could improve this animation, as these elements add additional detail about the morphology of polymers. In addition, being able to connect Maya prototype renderings to OpenGL (Open Graphics Library) for scientific visualization purposes could be accomplished with more time and resources. This link could help produce intuitive, realistic renderings of complex data from such simulation output.

Further study in polymer visualization should be explored, as this could potentially lead to more comprehensive perceptions and ultimately new discoveries in Polymer Science. For example, a group led by Dr. Ben Hsiao, a professor from State University of New York, has focused on the early stages of crystallization in polymer melts under shear flow. The group uses small angle X-ray scattering (SAXS) and wide-angle X-ray diffractions (WAXD) to investigate the molecular orientation at different melting temperatures in the polymer [SYZH05]. These oriented molecules, which contain primary nuclei that form shish-kebab structures, influence the crystallization kinetics and

the final morphology in the polymer. However, the early stages of crystallization are not fully understood due to the difficulty in performing precise experiments at these phases. Since the control of the nuclei topology is the key to altering the final morphology, producing such visualization through experimentation could assist Dr. Hsiao's group in performing experimentation at stages that were once thought to be impossible. This could enable scientists the ability to have more control of the crystallization process in any particular polymer.

REFERENCES

[BONN04] Daniel Bonn, Mathias Kobylko, Steffen Bohn, Jacques Meunier, Alexander Morozov, Wim van Saarloos, "Rod-Climbing Effect In Newtonian Fluids," November 2004.

[BRAN06] Lisa Brannon-Peppas, http://www.devicelink.com/mpb/archive/97/11/003.html, August 2006.

[BRYA03] Marc Bryant, "Interpreting Data: From Scientific Visualization to Visual Abstraction," Masters Thesis, Clemson University, August 2003.

[CAEF06] Center For Advanced Engineering Fibers and Film, http://caeff.ces.clemson.edu/, August 2006.

[CALL03] William D. Callister, Jr., Materials Science and Engineering: An Introduction, 2003, p.55.

[CART06] Dr. Sue Carter, http://physics.ucsc.edu/~sacarter/biosensor.shtml, August 2006.

[CLAS06] Classzone, http://www.classzone.com/books/earth_science/terc/content/investigations/es0506/es0506page01.cfm?chapter_no=investigation, August 2006.

[DAVI06] Michael Davidson, http://micro.magnet.fsu.edu/micro/gallery/polymer/polymer.html, August 2006.

[DISC06] Discover Media, http://www.discover.com/issues/oct-04/departments/observer/, August 2006.

[HSW06] How Stuff Works, http://health.howstuffworks.com/news-item186.htm, August 2006.

[HYLE06] Hyle, http://www.hyle.org/art/cia/index.html, October 2006.

[ILLI06] Paula Illingworth, http://www.usatoday.com/tech/news/techinnovations/2005-12-04-disaster-blanket_x.htm, August 2006.

[IV06] InVisu, http://www.invisu.ca/e/vuchem.php, October 2006.

[KROS87] Jacqueline I. Kroschwitz, An Encyclopedia Source Book of Engineering, 1987, p.449.

[MARK06] John Marko, http://www.lassp.cornell.edu/marko/polymers.html, August 2006.

[MBD06] Materials By Design, http://www.mse.cornell.edu/courses/engri111/skiing.htm, August 2006.

[MGL06] Molecular Graphics Laboratory, http://mgl.scripps.edu/people/goodsell/mgs_art/mgs_art2/index.html, October 2006.

[MIT06] Massachusetts Institute of Technology Website, http://web.mit.edu/ryeh/Public/die_swell.jpg, http://web.mit.edu/nnf/research/ phenomena/rod_climb_highres.jpg, August 2006.

[MOLE06] Molekel, http://www.cscs.ch/molekel/, October 2006.

[MW06] Merriam-Webster Online Dictionary, http://www.m-w.com/dictionary/, August 2006.

[OCTA06] Octa Project, http://octa.jp/index.html, August 2006.

[PARA06] Paraview, http://www.paraview.org/HTML/Index.html, http://www.paraview.org/Wiki/ParaView.Texture, http://www.paraview.org/Art/BigShot8.jpg, October 2006.

[PLCY06] Polymers and Liquid Crystals, http://plc.cwru.edu/tutorial/enhanced/files/polymers/apps/apps.htm, http://plc.cwru.edu/tutorial/enhanced/file/polymers/Orient/orient.htm, August 2006.

[PMM06] Erin Pytlik, Daryl Molino, Joseph Moritz, http://www.eng.buffalo.edu/Courses/ ce435/Diapers/Diapers.html, August 2006.

[POLI06] Polial, http://www.polial.polito.it/cdc/Mercurio/Polymer/mercurio_mechpro/07MP_MainConsdrns.htm#link_Viscoelasticity, August 2006.

[POLY06] Polymer Processing, http://www.polymerprocessing.com/feature/past/Y2000x09x01/page2.html, August 2006.

[PRN06] PRNewswire, http://www.prnewswire.com/cgi-bin/stories.pl?ACCT=104&STORY=/www/story/12-14-2000/0001387145&EDATE=, August 2006

[RRR00] Donald V. Rosato, M.G. Rosato, Dommick V. Rosato, Concise Encyclopedia of Plastics, 2000, p. 212.

[SYZH05] Rajesh H. Somani, Ling Yang, Lei Zhu, Benjamin S. Hsiao, "Flow-Induced Shish-kebab Precursor Structures in Entangled Polymer Melts," February 2005.

[TERA06] TeraGrid, http://hpcsoftware.teragrid.org/Software/user/show_all.php?deploy_id=477&view=TeraGrid, October 2006.

[TULL06] Alexander H. Tullo, http://pubs.acs.org/cen/coverstory/84/8424plastics.html, August 2006.

[VT06] Visualization Toolkit, http://www.vtk.org/, http://www.vtk.org/what-is-vtk.php, October 2006.

[WC06] Water Crystals, http://www.watercrystals.com, August 2006.

[WIKI06] Wikipedia, http://en.wikipedia.org/wiki/Tensile_strength, http://en.wikipedia.org/wiki/Image:Silly_putty_dripping.jpg, http://en.wikipedia.org/wiki/Maya_%28software%29#The_History_of_Maya, August 2006.